Supporting Information

Reversible Conductance Switching in Molecular Devices

By *Auke J. Kronemeijer, Hylke B. Akkerman, Tibor Kudernac, Bart J. van Wees, Ben L. Feringa, Paul W. M. Blom,* and *Bert de Boer**

[*] Prof. B. de Boer, A. J. Kronemeijer, H. B. Akkerman, Prof. B. J. van Wees, Prof. P. W. M. Blom
Zernike Institute for Advanced Materials, University of Groningen
Nijenborgh 4, 9747 AG Groningen (The Netherlands)
E-mail: b.de.boer@rug.nl
Dr. T. Kudernac, Prof. B. L. Feringa
Stratingh Institute for Chemistry, University of Groningen
Nijenborgh 4, 9747 AG Groningen (The Netherlands)

Computer Calculations of the SAM

The theoretically calculated layer thicknesses for a 0° tilt angle are 2.0 and 1.9 nm for the closed and open switches, respectively. This is done by calculating the end-to-end distance of the molecule using HyperChem 6.00 and including 2.3 Å for the Au–S bond (Figure 1). The energy of the molecule was minimized via geometrical optimization by using first Molecular Mechanics (method MM+) and secondly the semi-empirical method PM3 without configuration interactions. The geometrical optimization used the algorithm of Polak Ribiere (RMS gradient: 0.05 kcal/(Åmol)). The terminal S–H bond length was subtracted from the end-to-end distance and the Au–S distance of 2.3 Å was added.

Irradiation of the Devices

Illumination and consecutive measurements show that the characteristics of the closed switch are retrieved after 15 minutes UV irradiation of the open switch. Average values are calculated over at least 30 devices to gain statistics for reliable data. Irradiation at 532 nm for 45 minutes results in a decrease of the current densities through the devices. However, the characteristics of the complete open state are not achieved. Averages are taken over the same

devices (Figure 2). It is known that the quantum efficiency for ring opening of these switches is appreciably lower than for ring closure [1]. Therefore, the illumination time at 532 nm was set to 45 minutes to achieve ring opening of the switches in the SAM.

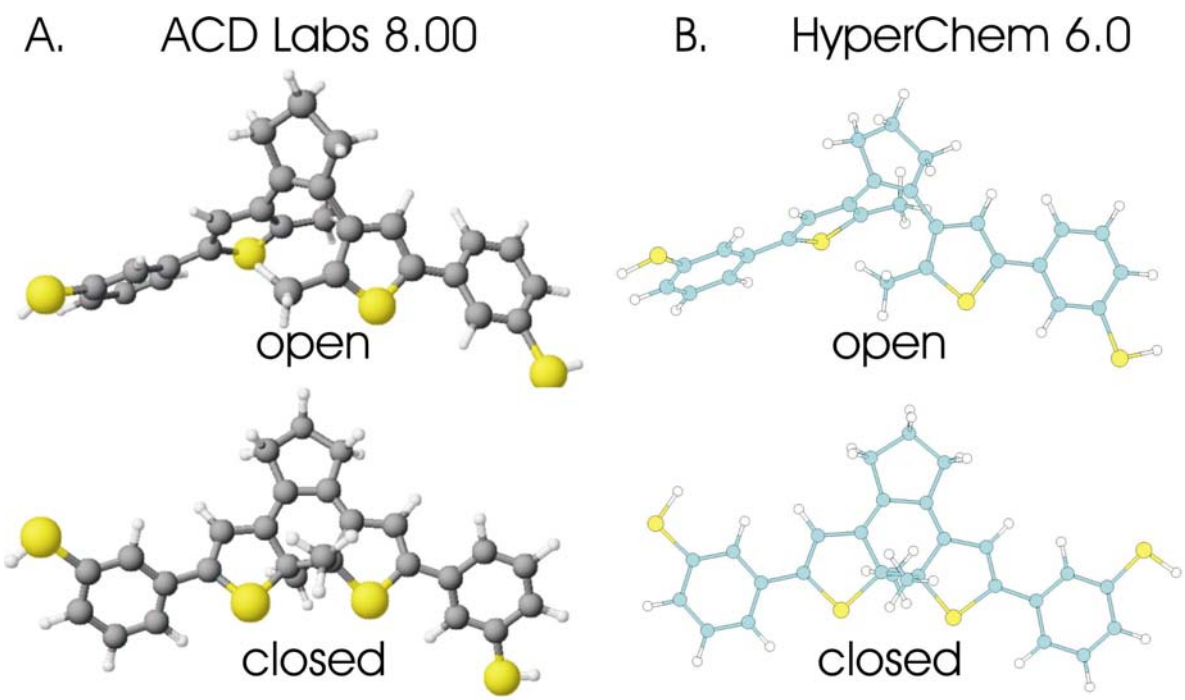

Figure 1: Computer modeling (A: with ACS Labs 8.00 software and B: with HyperChem 7.5) of the open and closed isomers demonstrates the planar structure for the closed isomer and the non-coplanar conformation for the open isomeric state.

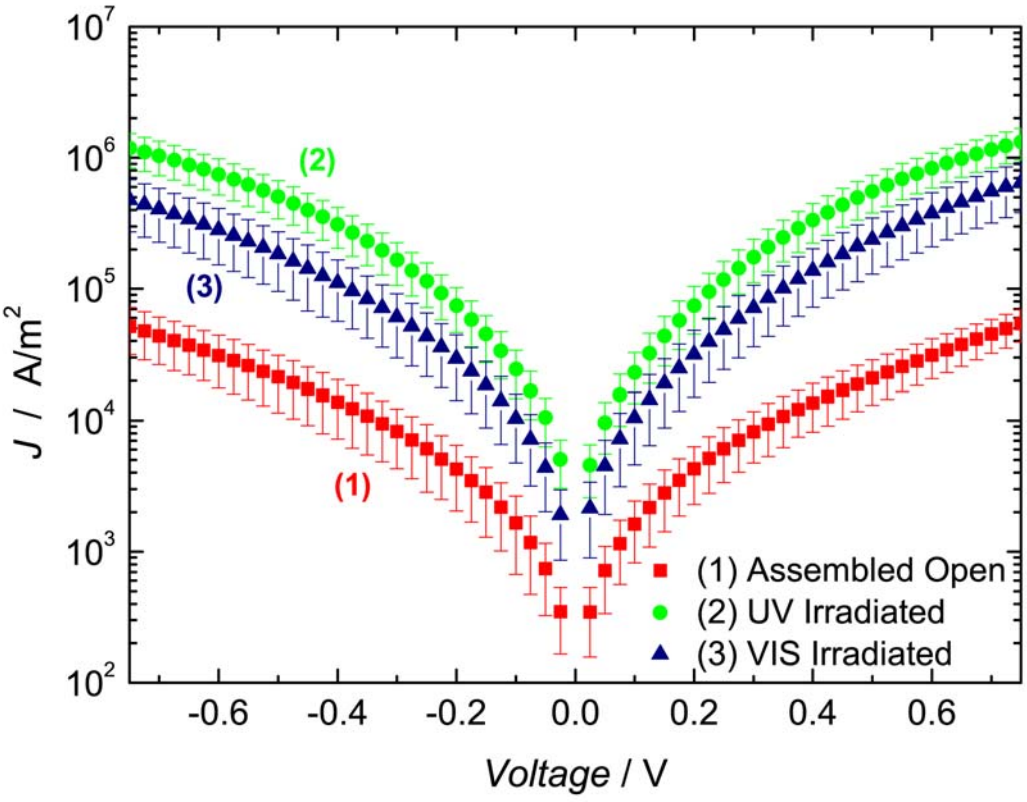

Figure 2: Electrical characteristics before and after UV illumination of the large-area molecular junctions. Error bars by standard deviation. UV illumination of devices with the open ring isomer self-assembled and consecutive visible irradiation of the same devices.

References:

[1] M. Irie, *Chem. Rev.* **2000**, *100*, 1685–1716.